1,1,2,3,3,3-Hexafluoro-1-propene 116-15-4 | DTXSID2026949

Model Performance

Model	Data
Model	Dala

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.87	0.81	0.87	0.82	0.86	0.86	

Model Results

Predicted value: 4.01e-04 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.45e-01

Confidence level: 5.81e-01

Nearest Neighbors from the Training Set

Image not found

Carbon tetrafluoride Measured: 2.14e-04 Predicted: 2.75e-04

Image not found

Ethane, hexafluoro-Measured: 5.64e-05 Predicted: 1.08e-04

Image not found

Cyclobutane, octafluoro-Measured: 1.65e-04 Predicted: 1.51e-04

Image not found

Bromotrifluoromethane Measured: 2.15e-03 Predicted: 2.18e-03

Image not found

Trifluoromethane Measured: 5.84e-02 Predicted: 3.40e-02